2-Butoxyethyl acetate

1	12-07-2	DTXSID	102690

Model Performance

M. J. I	D. L.
Model	Data
110001	Bata

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: -54.2 °C

Global applicability domain: Inside

Local applicability domain index: 7.66e-01

Confidence level: 6.26e-01

Nearest Neighbors from the Training Set

Image not found

2-Butoxyethyl acetate Measured: -63.0 Predicted: -54.2

Image not found

2-Ethoxyethyl acetate Measured: -61.7 Predicted: -56.7

Image not found

2-Ethoxyethyl acrylate Measured: -47.0 Predicted: -54.7

Image not found

2-Methoxyethyl acetate Measured: -70.0 Predicted: -63.1

Image not found

Dimethyl decanedioate

Measured: 38.0

Measured: 38.0 Predicted: 1.98